CONTENTS

Special Issue: Perspectives in Molecular Structure — A Collection of Invited Papers in Honour of Professor Bryce L. Crawford, Jr.

Preface ix
Spectroscopic studies of methane in collisions with rare gas atoms and diatomic molecules
K. Fox and D.E. Jennings (Greenbelt, MD, U.S.A.) 1
Vibrational studies of the disulfide group in proteins. Part II. Ab initio force fields and normal mode frequencies of dimethyl, methylethyl, and diethyl disulfides
W.-Y. Zhao and S. Krimm (Ann Arbor, MI, U.S.A.) 7
Electronic transitions of hydrogen bonded complexes: an electron energy loss spectroscopic study
T. Pradeep and C.N.R. Rao (Bangalore, India) 21
Vibrational modes of amorphous ice: bending mode frequencies for isotopically decoupled H_2O and HOD at 90 K
J.P. Devlin (Stillwater, OK, U.S.A.) 33
A non-adiabatic semi-empirical method for calculating the electron-vibrational spectra of large molecules. A possible approach for future studies
L.A. Gribov and V.I. Baranov (Moscow, U.S.S.R.) 45
Azines. Effect of basis set on calculated vibrational frequencies, infrared intensities and Raman intensities
K.B. Wiberg (New Haven, CT, U.S.A.) 61
The Raman scattering intesity parameters of acetylene
K.M. Gough and W.F. Murphy (Ottawa, Canada) 73
MO study of the monomer and adducts of dihydroxycarbene
R.L. Redington (Lubbock, TX, U.S.A.), C.W. Bock and B. Aboab (Marcus Hook, PA, U.S.A.) 89
Raman spectroscopic studies of polypyrrole on colloidal TiO_2: evidence for bipolarons
S. Umapathy and R.E. Hester (York, Gt. Britain) 113
Electronic current models of vibrational circular dichroism
L.A. Nafie and T.B. Freedman (Syracuse, NY, U.S.A.) 121
A new functional form for global potentials of floppy molecules
J.M. Bowman and P. Schafer (Atlanta, GA, U.S.A.) 133
A review of νCO bond-stretching wavenumbers for CO ligands in metal coordination compounds or clusters with emphasis on the less common types of metal/CO bonding patterns, and of the relationship between νCO and the internuclear distance, r(CO)
C. de la Cruz and N. Sheppard (Norwich, Gt. Britain) 141
Polarized Raman intensities of sodium formate crystal and its non-cylindrical electroopical parameters
H. Noma and K. Machida (Kyoto, Japan) 163
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part I. Environment effects on monomeric OH and self-associates
W.A.P. Luck and S. Peil (Marburg, F.R.G.) 175
IR studies of van der Waals interactions on perfluoro-t-butyl alcohol OH. Part II. Complexes with acetonitrile
W.A.P. Luck and S. Peil (Marburg, F.R.G.), L. Schriver and A. Schriver (Paris, France) 185
Normal coordinate analysis and force field of 18-crown-6
K. Fukuhara, K. Ikeda and H. Matsuura (Hiroshima, Japan) 203
Interpretation of infrared intensities. Part II. An intensity analysis, with applications to H_2O
W.B. Person and K. Kubulat (Gainesville, FL, U.S.A.) 225
Raman spectra of hydrated phospholipid bilayers. Part I. Measurement of humidity-dependent phase transitions
J.R. Scherer, S. Kint, B.A. Bolton and G.F. Bailey (Albany, CA, U.S.A.) 245

The concept of trigonal additivity
G. Raam Somayajulu and B.J. Zwolinski (College Station, TX, U.S.A.) 259
Dynamic infrared linear dichroism study of high-density and low-density polyethylene near the β-transition temperature
I. Noda, A.E. Dowrey and C. Marcott (Cincinnati, OH, U.S.A.) 265
Polarized Raman spectra of oriented all-*trans*-β-carotene in polyethylene films
G. Dellepiane, C. Cuniberti, R. Cavalli (Genoa, Italy), G. Masetti, E. Campani and G. Gorini (Pisa, Italy) 271
Tautomerism, protonation, and interaction with formiate, of phenyliminoimidazoline and benzylimidazolidine: AM1 and ab initio 4-31G calculations
J. Mavri and D. Hadži (Ljubljana, Yugoslavia) 285
Transient spectroscopy of a photochromic fulgide
D.A. Parthenopoulos and P.M. Rentzepis (Irvine, CA, U.S.A.) 297
Infrared and Raman spectra of hexaborides: force field calculations and isotopic effects
Z. Yahia, S. Turrell and G. Turrell (Villeneuve d'Ascq, France) and J.P. Mercurio (Limoges, France) 303
Structure determinations by MS, NMR and UV spectra of bromo and nitro derivatives of 1-azabenzanthrone
T. Ueda, Z. Abliz, M. Sato, M. Nishimura, S. Iwashima (Tokyo, Japan), J. Aoki (Chiba, Japan), T. Kan (Tokyo, Japan), S. Matsunaga and R. Tanaka (Osaka, Japan) 313
Conformational analysis, barriers to internal rotation, ab initio calculations and vibrational assignment for 1,1-dichloroacetone
J.R. Durig, J.A. Hardin and C.L. Tolley (Columbia, SC, U.S.A.) 323
Rotational isomerism of allylamine as studied by gas electron diffraction: a joint analysis with rotational constants and SCF MO calculation
Y. Hamada, M. Tsuboi, K. Yamanouchi, T. Matsuzawa and K. Kuchitsu (Tokyo, Japan) 345
Reaction of t-C_4H_9 with HI: possible negative activation energies
A.B. McEwen and D.M. Golden (Menlo Park, CA, U.S.A.) 357
Infrared intensities of CH stretching bands in partially deuterated compounds, and effects of conformation and substitution
A. Kindness, D.C. McKean and D. Stewart (Aberdeen, Gt. Britain) 363
An investigation of the vibrational spectra of glucose, galactose and mannose
H.A. Wells, Jr. and R.H. Atalla (Appleton, WI, U.S.A.) 385
Lattice dynamics and vibrational spectra of conformationally disordered polymers: poly(vinylidene fluoride)
G. Borionetti, G. Zannoni and G. Zerbi (Milan, Italy) 425
Infrared intensities: from intensity parameters to an overall understanding of the spectrum
M. Gussoni, M. Rui (Genoa, Italy), C. Castiglioni, G. Zerbi (Milan, Italy) and M.N. Ramos (Recife, Brazil) 445
High resolution Raman measurements of the temperature variation of the bandwidth of some lattice phonons and of one internal vibron of α-oxalic acid
N. van Tien, E. Castellucci, M. Becucci, S. Califano and D.A. Dows (Florence, Italy) 471

Author index 483
Subject index 485